School of Science and Mathematics

Student Research Poster Display

Caputo Hall Lobby

October 15—22, 2014

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Note: The names of Millersville University faculty advisors are designated by an asterisk (*) in the abstracts.

Biology

1. Identification of areas baited for *Odocoileus virginianus* using chemical analysis.

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Supplemental feeding and baiting of white-tailed deer has the potential to increase the spread of diseases such as Chronic Wasting Disease. Also, the baiting of wildlife for harvest is illegal in the state of Pennsylvania. The objective of this study was to determine if commercial deer baits leave a chemical signature in the soil that is detectable through chemical analysis. This information could then be used by conservation officers to determine if an area has had illegal baiting activity. Commercial deer baits were applied to experimental soil patches and compared to non-baited control soil patches. It was hypothesized that baited areas would exhibit elevated concentrations of calcium, sodium, and chloride compared to non-baited soil. Atomic absorption spectroscopy is being used to measure the concentration of sodium and calcium ions and a chloride probe will be used to measure chloride ions. Tentative results indicate that calcium is not an adequate indicator for baiting activity. Results also suggest that elevated levels of sodium are detectable in the baited areas. Therefore, detection of elevated levels of sodium could be used to determine if an area has been baited.

2. A Preliminary Study on Stream Restoration Effects on the Processing of Organic Matter

*Lukunich, Sara J. and Wallace, John R.**
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In general, invertebrates in freshwater systems are important mediators of the fragmentation of organic matter, thus influencing nutrient cycling and energy flow within stream food webs. In the last decade, those stream systems in Lancaster County significantly impacted by changes in land-use have been frequently restored in terms of channel design to alleviate suspended sediment and nutrient loading issues that impact downstream systems. This study was initiated to evaluate restoration effects on the macroinvertebrate community structure involved with processing organic matter (leaf packs). Leaf packs of dried tulip and oak leaves (4 gm/pack) were placed in riffle sections (n=6 packs/date) of the restored reach and a control stream and collected over a three-week period before restoration and 30 months after restoration. Packs were dried and weighed to determine rate of decomposition over time. Macroinvertebrates were identified to generic level to determine diversity and abundance. Preliminary results indicate that tulip leaves decomposed at a faster rate both pre and post restoration compared to oak leaf packs, but the rate did not differ between pre and post restoration. Macroinvertebrate diversity and abundance did not differ within sample years or between pre and post restoration. Often, post restoration monitoring of stream restoration projects does not continue much past restoration, and examining how they influence organic matter processing is completely ignored. This preliminary study provides much needed baseline data to assess how restoration may influence organic matter decomposition rates and potentially nutrient cycling and retention in a consumer-based system.

Biology

3. Impacts of Stream Restoration on Macroinvertebrate Community Structure and Adult Insect Recolonization on Big Spring Run (BSR), Lancaster County, PA.

*Neideigh, Emily C.; Smith, Robert F. (MU 1999); Rittle, Alex M. (MU 2013); Wallace, John R.**
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Because of the presence of an historic dam, Big Spring Run (BSR), located in Lancaster County, PA, and serves as a tributary to the Conestoga River, has been severely impacted by legacy sediment. By removing the legacy sediment, a section of BSR was restored with the objective of returning it to its natural floodplain. The purpose of this study was to examine how stream modification affects larval macroinvertebrate community structure as well as the abundance and diversity of recolonizing adult stream insects found along the restored section. Larval macroinvertebrates were collected late April-early May for two years pre-restoration and thirty-two months post-restoration using a BACI (Before/After/Control/Impact) sampling design to compare larval macroinvertebrate samples from three control sections to one restored section. Adult insects were collected using one malaise trap per stream site and sampled post-restoration only. Samples were identified to generic level in the lab for analysis. A nonmetric multidimensional scaling (NMDS) analysis was performed to compare macroinvertebrate communities while adult insects will be compared using the Simpsons Diversity Index. After thirty-two months post-restoration, our results indicated a significant improvement in the macroinvertebrate community structure in the restored section compared to previous post-restoration years. Early assessment of adult insect diversity and abundance reveals a trend of no difference among sites. Since results from stream restoration projects are not immediately observable and require post restoration monitoring, which many times is not included in the project design or cost, this project substantiates the importance of long-term monitoring and that not only macroinvertebrate communities but also recolonizing adults must be taken into account to determine if the projects met their stated objectives.

Chemistry

4. The Synthesis and Characterization of Indium Phosphide Quantum Dots For Use As Laser Diodes

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The study of quantum dots consisting of colloidal nanocrystal semiconductor particles in strong quantum confinement have become a very important topic of interest due to their applications in medical imaging, quantum computing, solar cells, and diode lasers. Indium phosphide quantum dots in particular have been used in laser diodes. The goal of this study is to synthesize indium phosphide quantum dots and characterize through: Tunneling Electron Microscopy, Ultraviolet-Visible Spectroscopy, and Fluorescence spectroscopy. These quantum dots will then be used to prepare a diode. Lastly, the diode will be prepared for use in a custom built laser.

5. Spectrophotometric Analysis of Cu in a Metal Ore

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Department of Chemistry, Millersville University, Millersville, PA 17551

A spectrophotometric method for determination of metal ions was developed and used to determine the amount of Cu in a copper ore. The goal of the work was to develop a laboratory experiment that integrates multiple concepts of interest in environmental and analytical chemistry courses. The simulated metal ore extract in a buffered solution was titrated with ethylenediammine tetracetic acid (EDTA). As the titration proceeded, the absorbance of the solution was measured using an Ocean Optics USB 4000 spectrophotometer. A plot of volume of titrant vs. absorbance showed two linear portions. The linear regression equation for each portion was determined and the two equations used to solve for the end point. The amount of Cu in the sample was then calculated taking into account stoichiometric ratios and dilution factors. The experiment developed reinforces multiple skills and concepts that are essential in analytical laboratory work.

6. Synthesis and Characterization of Catalytic Heterometallic Nanorods

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Metallic nanostructures are of great interest as heterogeneous catalysts due to their high surface area. The goal of this work was to synthesize core-shell Au-Ni nanorods for potential applications in green and sustainable chemical synthesis. Au-Ni nanorods were synthesized by a combination of template-assisted synthesis and galvanic replacement. Nickel was first electrodeposited by controlled potential electrolysis (CPE) in a porous alumina template coated with Ag on one side. Free standing nanorods were obtained by dissolving the Ag in 50% HNO_3 and the membrane in 2 M NaOH. Au was deposited on the Ni nanorods through a galvanic replacement reaction with 6 mM $HAuCl_4$. Preliminary studies show significant differences in the reduction of 2-nitrophenol by

Ni and Au nanorods, indicating that this reaction could be a suitable model system for investigating the relative catalytic activity of the heterometallic nanocatalysts.

7. Studies Toward the Synthesis of Hunanamycin A and its Derivatives

*John A. Noyes, James W. Dreer, Janelle B. Biehl, and Steven M. Kennedy**
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We have recently initiated studies toward the synthesize Hunanamycin A (HA). HA is a natural product first isolated from *Bacillus hunanensis*. It exhibits antibacterial activity for various pathogens such as *Salmonella* and *E. coli.* At the onset of this research project, conceivable synthetic routes to HA were designed based on related literature precedents for each planned reaction of the route. Currently, test reactions (*e.g.* nitration, reductive amination, and amine alkylation) are being optimized on model systems to explore multiple pathways of producing the target product, along with structurally similar derivatives, via chemical synthesis. Once an efficient synthetic route is elucidated, further biological testing of synthetic HA, and related derivatives, could allow for a calculated modification of the antibacterial properties displayed by this class of molecules. Our most progressive route to date employs a reductive amination method to provide a prenylated amine intermediate in moderate yield over multiple steps from commercially available and relatively inexpensive starting materials.

8. Progress toward an efficient synthesis of 1,1,3-trimethyl-3-phenylindan-4',5-dicarboxylic acid (PIDA): A Green Process.

*Omar, Mina and Bonser, Steven M.**
Department of Chemistry, Millersville University, Millersville, PA 17551

1,1,3-Trimethyl-3-phenylindan-4',5-dicarboxylic acid, commonly referred to as PIDA, is a polycondensation monomer used in industrial polyester polymerization processes. Although a number of syntheses of PIDA have been reported, a more environmentally friendly and cost effective process is desirable. The updated synthesis represents an efficient four-stage approach from readily available starting materials. The key step in the new reaction scheme is the use of "green" chemistry principles to oxidize the aryl methyl groups in 1,1,3,5-tetramethyl-3-(*p*-methylphenyl)indane to the corresponding dicarboxylic acid moieties of PIDA in the last step. The development of this optimized synthesis of PIDA is the subject of this poster.

Chemistry

9. Progress towards the synthesis of novel 3-aryl-3-chloro-1*H-diazirino*[1,2-*b*]phthalazine-3,8-diones.

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A long term goal in our laboratory is to develop some novel diaziridine compounds that may be useful intermediates to make a certain class of pharmaceutical; namely, the 2,4-benzodiazepines. We plan to utilize a new approach to synthesizing specific diaziridines that may provide a more

robust entry into the 2,4-benzodiazepine ring system. This new approach will exploit the reaction between certain chlorinated diaziridines with certain 1,2-diaroyl dichloride and 1,2-dibenzenesulfonyl dichloride compounds to generate the specific "designer“ diaziridines needed for this study. The progress of this study is the subject of this poster.

10. Heats of Formation of Energetic Compounds Using Computational Methods

*White, David L. and Elioff, Michael S.**
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We are conducting theoretical research related to finding gas-phase heats of formation for high energy density materials (HEDMs) using computational methods. HEDMs are compounds that detonate to produce large volumes of gas rapidly, and have a wide range of uses including mining, airbags, and military applications. These compounds have different structural considerations and encompass a large range of future potential materials. Our research is primarily aimed at finding appropriate and time-efficient methods for determining accurate heats of formation for eight compounds. The current methods being evaluated are Hartree Fock calculations and density functional theory (DFT) calculations using the B3LYP functional with at least 6-311G as the basis set. Previous studies into this subject have typically included factors for ring strain and steric interactions. We are examining the relationship between the connectivity of the atoms and the accuracy of the calculated energetic parameters.

Computer Science

11. Exploring the Theory of Algorithmic Self-Assembly

*Fansler, Mervin M.; Zoppetti, Gary M.**
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Self-assembly is a fundamental phenomenon in nature, expressing itself in crystal growth, viral replication, and cell reproduction. It is a process characterized by an automated assembly of subcomponents into a larger structure, often in a highly efficient and effective manner. In recent decades technology has advanced to the point of enabling the construction of arbitrary self-assembling systems on a nanoscale, with a broad potential for practical application. On the theoretical side, a number of models have emerged that have catalyzed advances in practical results, as well as stimulated a wealth of interdisciplinary research combining mathematics, computer science, chemistry and biology. Our research aims at surveying the present state of this field, in particular focusing on the theoretical computer science involved. Some of the topics being explored include the various models in use, the criteria necessary for universal computation, how algorithms manifest as patterns and structures in assemblies, and complexity analysis of assembly systems. An additional aim of this research is to identify some open problems in the field which could serve as candidates for undergraduate level thesis work.

Earth Sciences

12. Adapting to a Changing Climate at the NASA Wallops Flight Facility (WFF) & The Chincoteague Bay Field Station (CBFS)

*Nathan Murry and Ajoy Kumar**
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Wallops Island, VA is a largely undeveloped coastal ecosystem consisting of 18 barrier islands. As such, it is an excellent location for sustainability research, analysis of the effect of sea level rise on coastal ecology & municipal establishment, and the development of effective adaptation strategies for the NASA WFF, CBFS & surrounding areas. Our work uses remote sensing LiDAR (**Li**ght **D**etection and **R**anging) & satellite data to develop various digital models of the elevation & terrain (surface & bare-earth) of the NASA WFF & local vicinities. These digital models are used for extensive study of the scope & effect of inundation due to sea level changes on or around the NASA WFF in particular & the Eastern Shore in general.

Emergency Management

13. A Study of the Homeland Security Exercise and Evaluation Program with Special Examination of the Collaborative Planning Process

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Is emergency management exercise planning being conducted in a vacuum, where those who are trained in Homeland Security Exercise and Evaluation Program (HSEEP) act as gatekeepers for the exercise planning team members who are not HSEEP trained, especially with the loss of the HSEEP toolkit? This study uses an interview guide with open ended questions, a digital voice recorder, and a cellular telephone to interview thirty-two Master Exercise Practitioners from various fields with an advanced academic degree and/or the Certified Emergency Manager certification. Preliminary results are shared regarding the HSEEP guidance. The HSEEP guidance can be used to design strong exercises by a knowledgeable exercise director and committed planning team members, even without the toolkit. The guidance is a framework that can be adjusted to utilize several different formats, depending on the end user and organization. The HSEEP guidance is in line with most of the literature that covers exercise planning and collaboration.

Meteorology

14. Evaluating surface heat fluxes in the Ross Sea, Antarctica

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Millersville University & Old Dominion University

Atmospheric and oceanographic data collected during the 2012 PRISM (Processes Regulating Iron Supply at the Mesoscale) research cruise were used to construct surface heat budgets for three regions of the Ross Sea, Antarctica. Bulk method equations implemented used to determine net shortwave radiation, net longwave radiation, sensible heat flux, and latent heat flux. Net radiation had an observed range of -2 W m^{-2} to 88 W m^{-2} in the three locations. Sensible heat flux was the dominant term in the heat budget, ranging from -143 W m^{-2} to -9 W m^{-2}. Decreases in sensible heat flux of -143 W m^{-2} to -52 W m^{-2} correlated with increases in wind speed and decreases in ambient air temperature, indicating the occurrence of atmospheric events. The net heat loss following these events resulted in an overall heat loss from the ocean, suggesting that cooling during ice free conditions is regulated by episodic events. Climate projections predict that the Ross Sea will experience periods of ice free conditions in the coming decades. The results from this study suggest that this coupled with changes in atmospheric storm frequency could significantly alter the overall surface heat budget in the Ross Sea.

15. Temporal and Spatial Variability of Tropical Rain Rates over Kwajalein Atoll

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Precipitation extremes and how they may change in a future climate have potentially large regional impacts. The Intertropical Convergence Zone (ITCZ) produces a large amount of the rainfall in the tropics (and the globe). Located in the Pacific ITCZ and approximately nine degrees above the equator, Kwajalein Atoll was the base for NASA's ground validation of the Tropical Rainfall Measuring Mission (TRMM) satellite. Observations from the Kwajalein radar were manipulated using interface description language (IDL). The results highlight how topical precipitation extremes vary based on spatial resolution ranging from 2 km to 128 km, temporal resolution ranging from 10 minutes to 1 day, and rain type (i.e., convective vs. stratiform). The importance of stratiform rain (i.e., aged convection that is more horizontally homogeneous and with weaker rain rates than active convection) in the tropics is often not resolved by satellites and global climate models. The Kwajalein radar rain rate statistics are compared to TRMM precipitation radar (PR) retrievals to test the accuracy of the satellite rain rate distributions and are further separated by daily sea surface temperature (SST) and large-scale vertical motion at 500 hPa (i.e., the middle troposphere) to see how sensitive rain rates and precipitation extremes are to environmental parameters.

16. Verification of Earth Network's Dangerous Thunderstorm Alerts And National Weather Service Warnings

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The National Weather Center Research for Undergraduates Experience Program, Cooperative Institute for Mesoscale Meteorological Studies. NOAA/NWS/Warning Decision Training Branch and NOAA/OAR/National Severe Storms Laboratory.

Earth Networks Incorporated (ENI) has expressed the potential for their Dangerous Thunderstorm Alerts (DTAs) to increase lead time by an additional nine minutes over current National Weather Service (NWS) severe and tornado warnings while maintaining a similar probability of detection (POD) and False alarm ratio (FAR). These automated, storm-based alerts combine lightning-based storm tracking with total lightning flash rate thresholds to designate regions with an increased potential for severe and hazardous weather. ENI produces alert polygons at three different levels: (1) basic thunderstorm, (2) significant thunderstorm, and (3) dangerous thunderstorm. Verification statistics (including POD, FAR and lead time) for DTAs and NWS severe thunderstorm and tornado warnings are calculated for 20 May 2013 and for a year of data, March 2013 through Feb 2014, using StormData. The goal of this comparison is to reveal how well DTAs perform relative to NWS warnings and if use within operational meteorology will improve warnings. The results indicated that DTAs performed best in the convective season and performed comparably to NWS tornado warnings.

Meteorology

17. Effects of Wildfire Pollution on the Microphysical and Electrical Properties of Pyrocumulus

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Pyrocumulus clouds form over wildfires when hot, smoke-filled air rises, cools and condenses. These smoke-polluted clouds have higher cloud condensation nuclei (CCN) concentrations, which affect their microphysical and electrical properties. Lightning generation processes in pyrocumulus are not well understood, but have implications for wildfire growth predictions and the radiative and chemical characteristics of the upper troposphere (Lang et al. 2014). Lang et al. (2014) documented an electrified pyrocumulus over the May 2012 Hewlett Gulch fire outside of Fort Collins, Colorado, which produced approximately twenty intracloud lightning flashes. Motivated by their work, we investigate the microphysical differences between low CCN clean clouds and high CCN pyrocumulus. Model simulations were made of a cloud forming under five different CCN concentrations, ranging from clean to extremely polluted. Moderately polluted pyrocumulus experience a complete shutdown of rain processes and an increase in graupel production. In extremely polluted pyrocumulus, however, graupel production is halted, which allows for large amounts of liquid water and small ice. Using these microphysical details, a possible charging mechanism will be inferred and compared to Lang et al. (2014). The main goal is to better understand the aerosol-induced cloud-scale microphysics that causes pyrocumulus electrification to occur.

Physics

18. Detectability of Boulders on Near-Earth Asteroids

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Boulders are seen on spacecraft images of near-Earth asteroids Eros and Itokawa. Radar images often show bright pixels or groups of pixels that travel consistently across the surface as the object rotates, which may be indicative of similar boulders on other near-Earth asteroids. Examples of these bright pixels were found on radar observations of 2005 YU55 and 2006 VV2. One large possible boulder was found on on the surface of Bennu, target of the OSIRIS-REx sample return mission. We explore the detectability of boulders by adding synthetic features on asteroid models, and then simulating radar images. These synthetic features were added using BLENDER ver. 2.70, a free open-source 3-D animation suite. Starting with the shape model for Bennu (diameter ~500 m), spherical 'boulders' of 10 m, 20 m, and 40 m diameter were placed at latitudes between 0 and 90 deg. Simulated radar observations of these models indicated that spherical boulders smaller than 10 m may not be visible in observations but that larger ones should be readily seen. Boulders near the sub-Earth point can be hidden in the bright region near the leading edge, but as the asteroid's rotation moves them towards the terminator, they become visible again, with no significant dependence on the latitude of the boulder. These simulations suggest that we should detect large boulders under most circumstances in high-quality radar images, and we have a good estimate of the occurrence of such features on near-Earth objects.

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An asterisk (*) denotes the SCMA Faculty Advisor for the student research

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